

Entropy production in continuous phase space systems

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Abstract

We propose an alternative method to compute the entropy production of a classical underdamped nonequilibrium system in a continuous phase space. This approach has the advantage that it is not necessary to distinguish between even and odd-parity variables. We show that the method leads to the same local entropy production as in previous studies while the differential entropy production along a stochastic trajectory turns out to be different. This demonstrates that the differential entropy production in continuous phase space systems is not uniquely defined.

1 Introduction

In the past decade an important advance of nonequilibrium statistical physics has been the development of stochastic thermodynamics [1, 2]. In this approach thermodynamic quantities such as the entropy are defined as functionals along the microscopic stochastic trajectory of the system in its configuration space, allowing one to study fluctuations around the average. This led to the discovery of various fluctuation theorems which generalize the second law of thermodynamics [3–5]. For example, the total entropy S_{tot} of a system together with its environment in a nonequilibrium steady state is known to obey the integral fluctuation theorem $\langle e^{-\Delta S_{\text{tot}}} \rangle = 1$, implying the second law $\langle \Delta S_{\text{tot}} \rangle \geq 0$.

Discrete systems: The concept of stochastic thermodynamics is most easily introduced in the context of stochastic Markov jump processes. A Markov jump process is defined by a space of discrete classical configurations $c \in \Omega$ and certain transition rates $w_{c \rightarrow c'}(t) \geq 0$ for spontaneous jumps from c to c' . As time evolves, such a system jumps randomly in its own configuration space, producing a stochastic trajectory

$$\gamma : c_0 \rightarrow c_1 \rightarrow c_2 \rightarrow \dots \quad (1)$$

of instantaneous transitions taking place at certain transition times $t = t_1, t_2, \dots$

In stochastic thermodynamics it is assumed that the total entropy can be written as a sum of the internal entropy of the system and the entropy of the environment

$$S_{\text{tot}}(t) = S_{\text{sys}}(t) + S_{\text{env}}(t). \quad (2)$$

The internal entropy $S_{\text{sys}}(t)$ is a fluctuating quantity defined by

$$S_{\text{sys}}(t) = -\ln p_{c(t)}(t), \quad (3)$$

where $p_c(t)$ denotes the probability to find the system in the configuration c at time t . Since this probability evolves deterministically according to the master equation

$$\dot{p}_c(t) = \sum_{c' \in \Omega} [p_{c'}(t)w_{c' \rightarrow c}(t) - p_c(t)w_{c \rightarrow c'}(t)] \quad (4)$$

the internal entropy $S_{\text{sys}}(t)$ evolves smoothly superposed by discontinuous jumps whenever the system hops to a different configuration. Averaging $S_{\text{sys}}(t)$ over the probability distribution $p_c(t)$ one retrieves the usual Boltzmann-Gibbs or Shannon entropy

$$\langle S_{\text{sys}}(t) \rangle = -\sum_c p_c(t) \ln p_c(t). \quad (5)$$

Nonequilibrium systems are usually driven from outside, i.e. they interact with the environment. On the level of the Markov process the environment is usually not modeled explicitly, rather it is implemented implicitly by means of asymmetric rates ($w_{c' \rightarrow c} \neq w_{c \rightarrow c'}$). For example, a system describing the flow of heat between two reservoirs at different temperatures is usually described in terms of a biased diffusion process which drives the particles on average in one direction. In a nonequilibrium steady state the internal entropy $\langle S_{\text{sys}}(t) \rangle$ of such a system will be on average constant, but the incessant external drive will continually increase the entropy in the environment. Remarkably, the external entropy production $\dot{S}_{\text{env}}(t)$ can be quantified even if the physical properties of the environment are not known. In fact, as shown in [4, 9], whenever the system hops from c to c' , S_{env} changes discontinuously by the amount

$$\Delta S_{\text{env}} = \ln \frac{w_{c \rightarrow c'}(t)}{w_{c' \rightarrow c}(t)}, \quad (6)$$

irrespective of the physical realization of the environment.

Overdamped continuous systems: The entropy production for *overdamped* Langevin systems in a continuous state space is defined in same spirit. Let us, for example, consider the Langevin equation of a single particle

$$\dot{x} = \mu F(x, t) + \zeta(t), \quad (7)$$

where $F(x, t)$ is a force, $\zeta(t)$ is a white Gaussian noise with temporal correlations $\langle \zeta(t)\zeta(t') \rangle = 2D\delta(t-t')$, and $\mu = D/T$ is the mobility of the particle. Monitoring the particle coordinate up to time T , each stochastic path $\gamma = \{x(t)\}$ starting at position x_0 will occur with a certain probabilistic weight $\mathcal{P}[\gamma|x_0]$. In this situation the entropy production in the environment is given by [5]

$$\Delta S_{\text{env}} = \ln \frac{P[\gamma|x_0]}{P^\dagger[\gamma^\dagger|x_0^\dagger]}, \quad (8)$$

where the symbol \dagger denotes the operation of path reversal $x^\dagger(t) = x(T-t)$, combined with the exchange of final and initial position $x_0^\dagger = x_T$ and the reversal of the protocol $t \rightarrow T-t$ for time-dependent forces (corresponding to time-dependent rates in the discrete case). Obviously, this expression is just a continuum version of Eq. (6), where the positions x play the same role as the configurations c in the discrete case.

It is important to note that the operation \dagger does not involve a *physical* time reversal operation, i.e. there is nothing “running backward in time”. In fact, γ^\dagger is just the reflected path and $P^\dagger[\gamma^\dagger|x_0^\dagger]$ its statistical weight in the *same* physical process running forward in time, only using a reflected protocol in the case of time-dependent transition rates.

Underdamped continuous systems: In the *underdamped* case, however, the situation is more complicated. Here the state of a particle is characterized by positions q and momenta p . Considering (q, p) as a configuration and reversing a stochastic trajectory naively by replacing

$$\gamma = \{q(t), p(t)\} \longrightarrow \gamma_{\text{naive}}^\dagger = \{q^\dagger(t), p^\dagger(t)\} = \{q(T-t), p(T-t)\} \quad (9)$$

would result into a conjugate trajectory running backward in space but with the velocity pointing in the wrong direction. This problem can be overcome by either an additional explicit reflection of time $t \rightarrow -t$, which means γ^\dagger is actually running backward in time, or – formally equivalent – by redefining the \dagger -operation in such a way that it changes the sign of p by itself. Using the latter approach Spinney and Ford (SF) introduced a general formalism that distinguishes between odd and even variables under the \dagger -operation [6], i.e.

$$\gamma = \{q(t), p(t)\} \longrightarrow \gamma^\dagger = \{q^\dagger(t), p^\dagger(t)\} = \{\epsilon q(T-t), \epsilon p(T-t)\} \quad (10)$$

with $\epsilon = +1$ for q and $\epsilon = -1$ for odd quantities such as p . Using this formalism Spinney and Ford were able to compute the entropy production of arbitrary Langevin systems with inertia, in particular for *underdamped* equations of motion in the full (q, p) phase space.

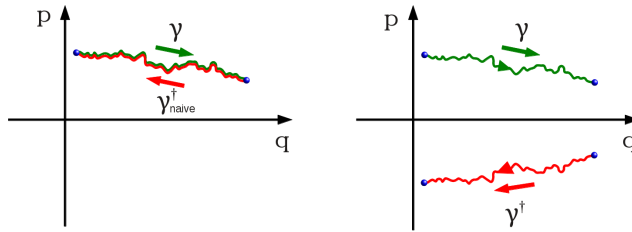


Figure 1: [Color online] Path reversal in phase space. Left: Reversing the trajectory naively by replacing $t \rightarrow T - t$ leads to an unphysical path where momentum and velocity are oriented in opposite direction. Right: Path conjugation proposed by Spinney and Ford, flipping in addition the sign of the momentum.

However, it remains unsatisfactory that the redefined \dagger -operation maps the trajectory γ to a completely different part of phase space, where the physical properties of the process could be potentially different (see Fig. 1). As for the terminal points of the trajectory, instead of simply exchanging x_0 with x_T , one substitutes $(q_0, p_0) \rightarrow (q_T, -p_T)$ and $(q_T, p_T) \rightarrow (q_0, -p_0)$, the two terminal points are replaced with a *different* pair of points, which seems to be in contradiction with the spirit of Eq. (6). We believe that this circumstance plays a role in the context of the so-called *odd-parity variable problem* which is currently discussed in the community [14].

In the present paper we demonstrate that the strict distinction between odd and even variables is not needed in order to define a physically meaningful entropy production. Following the spirit of Seiferts approach in Ref. [5] we define the differential entropy production by a logarithmic ratio of the weights of two forward processes, identifying the underlying Hamiltonian orbits as the microscopic states of the system. This approach is simpler as it is no longer necessary to distinguish between even and odd variables. Moreover, it is possible to consider Langevin equations with arbitrary functions which are neither symmetric nor antisymmetric. Surprisingly we find that the differential entropy production differs from the one computed by Spinney and Ford. However, evaluating physical quantities both forms of the differential entropy yield exactly the same result, meaning that the two approaches are equivalent. Therefore, we arrive at the conclusion that the differential entropy production is to some extent ambiguous, meaning that different expressions can describe the same physical situation.

2 Definitions and Notations

In what follows we study a particle with phase space coordinates $(q(t), p(t))$ in a potential $V(q)$ which is in contact with an external heat bath. The stochastic

trajectory of the particle is described by the Langevin equation

$$\dot{q} = p, \quad \dot{p} = -V'(q) - \gamma(p)p + \Gamma(p)\xi. \quad (11)$$

Here $\xi(t)$ denotes a white Gaussian noise with correlations $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$ which is understood to be integrated in the Itô sense throughout this paper. For simplicity we set the mass of the particle to $m = 1$. In order to include the possibility of nonlinear friction the coefficient $\gamma(p)$ and the noise amplitude $\Gamma(p)$ are assumed to be p -dependent functions. In the simplest case of linear friction the coefficients γ and Γ are constant and obey the Einstein relation $\Gamma = \sqrt{2T\gamma}$.

Fokker Planck equation: Following Ref. [8] and using the vector notation $\mathbf{x} = (q, p)$ the Langevin equation (11) can be written as a stochastic differential equation of the form

$$d\mathbf{x}_i = A_i(\mathbf{x}, t)dt + B_i(\mathbf{x}, t)dW_i, \quad (12)$$

where dW_i denotes the Wiener process generated by the noise $\xi(t)$. For Itô integration, the probability distribution $P(\mathbf{x}, t)$ to find the particle in the phase space point $\mathbf{x} = (q, p)$ at time t evolves according to the Fokker Planck equation

$$\partial_t P(\mathbf{x}, t) = - \sum_i \partial_{x_i} J_i(\mathbf{x}, t), \quad (13)$$

where

$$J_i(\mathbf{x}, t) = A_i(\mathbf{x}, t)P(\mathbf{x}, t) - \partial_{x_i} [D_i(\mathbf{x}, t)P(\mathbf{x}, t)] \quad (14)$$

is the dynamical probability current with the diffusion coefficients

$$D_i(\mathbf{x}, t) = \frac{1}{2} B_i(\mathbf{x}, t)^2. \quad (15)$$

More specifically, for the Langevin equation (11) describing a single particle in a potential $V(q)$ the Fokker-Planck equation (13) is given by

$$\begin{aligned} \partial_t P(q, p, t) = & \left([\gamma(p) + p\gamma'(p) + \Gamma(p)\Gamma''(p) + \Gamma'(p)^2] \right. \\ & + [p\gamma(p) + 2\Gamma(p)\Gamma'(p) + V'(q)] \partial_p \\ & \left. + \frac{1}{2} \Gamma(p)^2 \partial_p^2 - p \partial_q \right) P(q, p, t). \end{aligned} \quad (16)$$

Generalized Einstein relation: For a single particle in a heat bath the Langevin equations (11) can be split into a component given by the Hamilton equations of motion with the Hamiltonian $\mathcal{H}(q, p) = p^2/2 + V(q)$ and a component $-\gamma(p)p + \Gamma(p)\xi$ accounting for the heat bath. Of particular interest are

dynamical rules for which the system evolves into a stationary Boltzmann-Gibbs distribution of the form

$$p_{\text{eq}}(q, p) = \frac{e^{-\beta \mathcal{H}(q, p)}}{Z} = \frac{1}{Z} \exp \left[-\beta \left(\frac{p^2}{2} + V(q) \right) \right], \quad (17)$$

where $\beta = 1/T$ and $k_B := 1$. Inserting this distribution on the r.h.s. of the Fokker-Planck equation one obtains a first-order differential equation in $\gamma(p)$ with the solution

$$\gamma(p) = \frac{1}{2} \beta \Gamma(p)^2 - \frac{\Gamma(p) \Gamma'(p)}{p} + \frac{C e^{\frac{\beta p^2}{2}}}{p}, \quad (18)$$

where C is an integration constant. Since the last term would lead to a divergent mean acceleration of the particle in the stationary state, it is unphysical so that we have to set $C = 0$. The remaining expression

$$2p\gamma(p) = \beta p \Gamma(p)^2 - 2\Gamma(p) \Gamma'(p) \quad (19)$$

relates the noise amplitude $\Gamma(p)$ with the friction coefficient $\gamma(p)$, generalizing the Einstein relation $2\gamma = \beta \Gamma^2$ for linear dissipation and additive noise.

Short-time propagator: An important function that will be needed to compute the differential entropy production in the following section is the short-time propagator $G(\mathbf{x}'|\mathbf{x}; dt)$ of the Fokker-Planck equation. The short-time propagator can be understood as the probability density to find a particle starting from position \mathbf{x} at the position \mathbf{x}' after an infinitesimal time span dt .

Since the short-time propagator has to solve the Fokker Planck equation only to lowest order in dt it is not uniquely defined [10, 11]. The origin of this ambiguity is two-fold. On the one hand, the *form* of the propagator function does not need to be Gaussian because the central limit theorem guarantees that any distribution with the correct first and second moment will lead to the same macroscopic propagator. On the other hand, there is an additional freedom in choosing the evaluation point of the amplitudes $A_i(\mathbf{x}, t)$ and $D_i(\mathbf{x}, t)$: These functions need not necessarily be evaluated at the starting position \mathbf{x} of the propagator but they could also be evaluated at the final position \mathbf{x}' or at any position in the immediate neighborhood of these points. Of course, this would generate corrections which have to be compensated to lowest order by suitable counterterms in the propagator. Although this freedom reminds one of the Itô-Stratonovich dilemma we emphasize that this ambiguity is an additional freedom which is completely independent of our choice to use the Itô scheme in the Langevin equation.

Following Ref. [8] we will consider a subspace of all possible solutions by introducing a parameter $a \in [0, 1]$ and defining the short-time propagator by

$$G_a(\mathbf{x}'|\mathbf{x}; dt) = \prod_i (4\pi D_i dt)^{-1/2} \times \exp \left[-\frac{(dx_i - A_i dt + 2aD'_i dt)^2}{4D_i dt} - aA'_i dt + a^2 D''_i dt \right], \quad (20)$$

where the functions and their partial derivatives

$$\begin{aligned} A_i &= A_i(\mathbf{r}, t), & A'_i &= \partial_{r_i} A_i(\mathbf{r}, t), \\ D_i &= D_i(\mathbf{r}, t), & D'_i &= \partial_{r_i} D_i(\mathbf{r}, t), & D''_i &= \partial_{r_i}^2 D_i(\mathbf{r}, t) \end{aligned}$$

are evaluated at the point $\mathbf{r} = (1-a)\mathbf{x} + a\mathbf{x}'$ on a straight line between the two points \mathbf{x} and \mathbf{x}' . It is straight forward to verify that this propagator solves the Fokker-Planck equation to first order in dt .

Short-time propagator for an underdamped particle: The underdamped particle in Eq. (11) is described by a system of two differential equations, namely, a deterministic equation $\dot{q} = p$ and a SDE for \dot{p} . To compute the short-time propagator we first add an infinitesimally small noise in the first component, i.e. we consider the Langevin equations

$$\dot{q} = p + \epsilon \xi_q, \quad \dot{p} = -V'(q) - \gamma(p)p + \Gamma(p)\xi_p \quad (21)$$

with two uncorrelated Gaussian noise functions $\xi_q(t)$ and $\xi_p(t)$

$$\begin{aligned} G_a^\epsilon(q', p'|q, p; dt) &= \frac{1}{2\pi\epsilon\Gamma(r)dt} \exp \left[a^2 \left(\Gamma(r)\Gamma''(r) + \Gamma'(r)^2 \right) dt \right. \\ &\quad - \frac{\left(V'(q + adq)dt + 2a\Gamma(r)\Gamma'(r)dt + dp + r\gamma(r)dt \right)^2}{2\Gamma(r)^2 dt} \\ &\quad \left. + a(r\gamma'(r) + \gamma(r))dt - \frac{(dq - r dt)^2}{2\epsilon^2 dt} \right], \end{aligned} \quad (22)$$

where $dq = q' - q$, $dp = p' - p$, and

$$r = r(p, p') = p + a(p' - p) \quad (23)$$

is the momentum at which the functions are evaluated. As expected, by taking $\epsilon \rightarrow 0$ we obtain

$$G_a(q', p' | q, p; dt) = \frac{\delta(dq - r dt)}{\sqrt{2\pi dt} \Gamma(r)} \exp \left[a^2 \left(\Gamma(r) \Gamma''(r) + \Gamma'(r)^2 \right) dt \right. \\ \left. - \frac{\left(V'(adq + q)dt + 2a\Gamma(r)\Gamma'(r)dt + dp + r\gamma(r)dt \right)^2}{2\Gamma(r)^2 dt} \right. \\ \left. + a(r\gamma'(r) + \gamma(r)) dt \right] \quad (24)$$

which is deterministic in the position coordinate.

3 Differential entropy production

The differential entropy dS_{env} can be understood as a Taylor expansion of ΔS_{env} to lowest order in dq , dp and dt along an infinitesimal line element of the trajectory γ in phase space. In the following we show that this differential entropy production can be defined in different ways.

Differential entropy production according to Spinney and Ford: As already outlined in the Introduction, the amount of entropy generated in the environment along a stochastic trajectory γ is given by

$$\Delta S_{\text{env}} = \ln \frac{P[\gamma | \mathbf{x}_0]}{P^\dagger[\gamma^\dagger | \mathbf{x}_0^\dagger]}. \quad (25)$$

where \dagger stands for a suitable path conjugation operation. As suggested by Spinney and Ford [6], this conjugation has to change the sign of odd-parity variables such as momenta, i.e.

$$\gamma : (q_0, p_0) \rightarrow (q_T, p_T) \quad \xrightarrow{\dagger} \quad \gamma^\dagger : (q_T, -p_T) \rightarrow (q_0, -p_0). \quad (26)$$

Using this definition of path reversal, the *differential* entropy production according to Spinney and Ford (see Eq. (25) of Ref. [8]) along an infinitesimal section of a path is given by

$$dS_{\text{env}}^{\text{SF}} = \ln \frac{G_a(\mathbf{x}' | \mathbf{x}; dt)}{G_b(\mathbf{x}'^\dagger | \mathbf{x}^\dagger; dt)}, \quad (27)$$

where a, b are free parameters reflecting the ambiguity of the short-time propagator. In the special case of the underdamped particle Eq. (21) we have

$$dS_{\text{env}}^{\text{SF}} = \lim_{\epsilon \rightarrow 0} \ln \frac{G_a^\epsilon(q', p' | q, p; dt)}{G_b^\epsilon(q, -p | q', -p'; dt)}. \quad (28)$$

Clearly, the limit $\epsilon \rightarrow 0$ can only be carried out if the two propagators peak at the same position in phase space. Roughly speaking this means that the two δ -functions (see Eq. (24)) have to cancel out when taking the limit individually in the propagators since otherwise the entropy production would be locally divergent. This leads directly to the condition

$$(q' - q) - (p + a(p' - p))dt = -[(q - q') - (-p' + b(-p + p'))dt] \quad (29)$$

with the solution $b = 1 - a$, replacing a lengthy derivation in the appendix of Ref. [8]. Setting $a = 0$ and $b = 1$ Spinney and Ford expanded the differential entropy production to first order in dt and to second order in dp , arriving at

$$\begin{aligned} dS_{\text{env}}^{\text{SF}} = & \frac{1}{\Gamma^2} \left(-\gamma\Gamma^2 - \Gamma^3\Gamma'' + \Gamma^2\Gamma'^2 - \Gamma^2p\gamma' + 2\gamma\Gamma p\Gamma' - 2\gamma pV' - 2\Gamma\Gamma'V' \right) dt \\ & + \frac{1}{\Gamma^2} \left(-2\Gamma\Gamma' - 2\gamma p \right) dp + \mathcal{O}(dt^2) + \mathcal{O}(dp^3), \end{aligned} \quad (30)$$

where for the sake of brevity we dropped the arguments of the functions $\Gamma(p)$, $\gamma(p)$, and $V(q)$ which are all evaluated at the point (q, p) .

Although all the final results derived by Spinney and Ford eventually turn out to be correct and physically plausible, the differential entropy production given above has surprisingly implausible properties. For example, for a free particle ($V = 0$) subjected to linear friction ($\gamma(p) = \gamma = \text{const}$) in thermal equilibrium with a heat bath ($\Gamma = \sqrt{2T\gamma}$) the above expression reduces to

$$dS_{\text{env}}^{\text{SF}} = -\beta p dp - \gamma dt. \quad (31)$$

This means that a resting particle ($p = 0$) continually produces negative entropy in the environment. This is surprising since in the discontinuous case a system resting in a particular configuration does not produce any entropy. In fact, this observation was the starting point that motivated the present work.

On the meaning of points in phase space: In the arguments given above and in most papers about entropy production in continuous systems, it is implicitly assumed that the configurations c in the discrete case should correspond to individual points in phase space, i.e. the points in phase space are identified as the ‘microstates’ of the system. However, as we will argue in the following, it is not clear whether such a simple identification is correct.

To see this, let us disconnect the external reservoir (in our example by setting $\gamma(p) = \Gamma(p) = 0$). What is left over is a classical Hamiltonian system which does not produce entropy in the environment, analogous to a discrete system which stays in a single configuration c . However, the disconnected Hamiltonian system

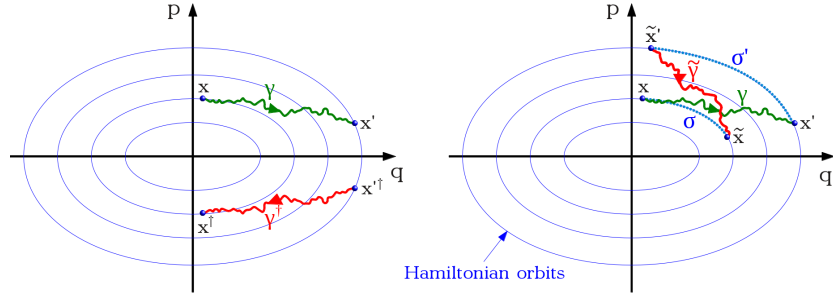


Figure 2: [Color online] Two different schemes to define the conjugate path. Left: Spinney's and Ford's approach mirrors the terminal points at the q -axis into a different part of phase space. Right: In our approach the terminal points are instead exchanged along the underlying Hamiltonian orbits σ and σ' .

does not stay in a single point, instead it still moves along its deterministic trajectory given by the Hamiltonian equations of motion. This leads us to the conjecture that all points *connected by the Hamiltonian flow* should be considered as belonging to the same 'microstate' of the system. In other words, we suggest that the 'microstates' of the system are the underlying Hamiltonian orbits rather than individual points in phase space.

Reconnecting the system with the external reservoir, the thermal noise will permanently drive the system away from one Hamiltonian orbit to another. We suggest that such a thermally induced change of the Hamiltonian orbit can be interpreted as a spontaneous jump to a different 'microstate', analogous to a change of the configuration $c \rightarrow c'$ in the discrete case. This would imply that only transitions between different Hamiltonian orbits should change the entropy in the environment, opposed to the formula (2) suggested by Spinney and Ford.

Differential entropy production based on Hamiltonian orbits: In what follows we propose a new definition of environmental entropy production with respect to the Hamiltonian orbits instead of points in phase space. This definition does not require parity operations, meaning that it is not necessary to distinguish between odd and even variables. As we will see, this leads in fact to a different expression for the differential entropy production. However, after integration we are led to exactly the same physical predictions as Spinney and Ford, suggesting that the definition of the differential entropy production is not unique.

Our method is applicable to systems which can be separated into a Hamiltonian part and another contribution coming from the external environment so that it is possible to identify the underlying Hamiltonian orbits, denoted here

by σ .

Our approach is motivated as follows: As shown in Fig. 2, a given stochastic path γ typically connects two different underlying Hamiltonian orbits σ and σ' . According to the arguments given above, the conjugate path, which is denoted here by $\tilde{\gamma}$ (in order to distinguish it from γ^\dagger used by Spinney and Ford), should run from σ' to σ in such a way that the terminal points of the trajectories are crosswise connected by the Hamiltonian flow (see Fig. 2). This ensures that both γ and $\tilde{\gamma}$ are defined as forward trajectories in the *same* part of phase space so that the special treatment of odd variables is no longer necessary:

path	transition	starting point	ending point
γ	$\sigma \rightarrow \sigma'$	$\mathbf{x} = (q, p)$	$\mathbf{x}' = (q', p')$
$\tilde{\gamma}$	$\sigma' \rightarrow \sigma$	$\tilde{\mathbf{x}} = (\tilde{q}, \tilde{p})$	$\tilde{\mathbf{x}}' = (\tilde{q}', \tilde{p}')$

Using this conjugation scheme, we define the differential entropy production as

$$dS_{\text{env}}^{\text{HF}}(\mathbf{x}'|\mathbf{x}; dt) = \ln \frac{G_a(\mathbf{x}'|\mathbf{x}; dt)}{G_b(\tilde{\mathbf{x}}|\tilde{\mathbf{x}}'; dt)}, \quad (32)$$

where the phase space points \mathbf{x} and $\tilde{\mathbf{x}}$ (and likewise $\tilde{\mathbf{x}}'$ and \mathbf{x}') are connected by the Hamiltonian flow (HF) over the time span dt . The parameters a, b reflect the ambiguity of the short-time propagator and will be determined later. Moreover, we dropped a possible explicit time dependency of the propagator.

Application to a single particle: In the example of a single underdamped particle, we have

$$\tilde{\mathbf{x}} = (\tilde{q}, \tilde{p}) = (q + p dt, p + f(q) dt) \quad (33)$$

$$\tilde{\mathbf{x}}' = (\tilde{q}', \tilde{p}') = (q' - p' dt, p' - f(q') dt) \quad (34)$$

so that

$$dS_{\text{env}} = \lim_{\epsilon \rightarrow 0} \ln \frac{G_a^\epsilon(q', p' | q, p; dt)}{G_b^\epsilon(q + p dt, p + f(q) dt | q' - p' dt, p' - f(q') dt; dt)}. \quad (35)$$

Again this expression can only be evaluated if the singularities arising in the limit $\epsilon \rightarrow 0$ cancel out, leading to the condition

$$\begin{aligned} & (q' - q) - (p + a(p' - p)) dt \\ &= - \left[(q - q') + (p + p') dt - (p' - f(q') dt + b(p - p' + (f(q) + f(q')) dt) \right] \end{aligned} \quad (36)$$

Expanding the force by $f(q') = f(q) + f'(q)(q' - q) + \mathcal{O}(dt^2)$ and neglecting terms of the order dt^3 this equation is solved for $a = b = 1/2$. This result is very plausible: It simply means that the functions appearing in the two propagators have to be evaluated at the same point in phase space. In the case considered by Spinney and Ford, apart from the reflection in the momenta, this means that the position coordinates have to coincide, giving $a = b$. In our method, however, this happens only at the particular point where the two trajectories cross each other, namely, roughly in the middle of the four points $(\mathbf{x}, \mathbf{x}', \tilde{\mathbf{x}}, \tilde{\mathbf{x}}')$.

Inserting $a = b = 1/2$ the differential entropy production suggested by us is given by

$$\begin{aligned} dS_{\text{env}}^{\text{HF}} = & \frac{1}{\Gamma^2} \left(-2p\gamma V' - 2\Gamma\Gamma'V' \right) dt + \frac{1}{\Gamma^2} \left(-2p\gamma - 2\Gamma\Gamma' \right) dp \\ & + \frac{1}{\Gamma^2} \left(-p\gamma' + \frac{2p\gamma\Gamma'}{\Gamma} - \gamma - \Gamma\Gamma'' + \Gamma'^2 \right) dp^2 + \mathcal{O}(dt^2) + \mathcal{O}(dt^3), \end{aligned} \quad (37)$$

where we again dropped the arguments of the functions $\Gamma(p), \gamma(p)$, and $V(q)$ which are all evaluated at the point (q, p) . Obviously, this differential entropy production is different from the one in Eq. (30) proposed by Spinney and Ford:

- In contrast to their result, our differential entropy production vanishes to first order in dt along the deterministic trajectory $dp = -V'(q)dt$.
- While Spinney and Ford's expression is linear in dt and dp , our version includes also a second-order term dp^2 .
- In our case the differential entropy production of a resting free particle vanishes while it is non-zero in the Spinney-Ford case (see Eq. (31)).

4 Local entropy production rate

Definition: The local entropy production rate \dot{S}_{env} is defined as the temporal derivative of the integral over the differential entropy production of all paths originating at the point \mathbf{x} weighted with the corresponding probability of the path:

$$\dot{S}_{\text{env}}(\mathbf{x}) = \lim_{dt \rightarrow 0} \frac{1}{dt} \int_{-\infty}^{+\infty} d\mathbf{x}' G_c(\mathbf{x}'|\mathbf{x}; dt) dS_{\text{env}}(\mathbf{x}'|\mathbf{x}; dt), \quad (38)$$

where $c \in [0, 1]$ is another free parameter which reflects the ambiguity in the short-time propagator. Note that this parameter is independent of the parameters a, b appearing in the differential entropy production and also independent of the integration scheme used in the Langevin equation.

In the example of a single particle we have

$$\dot{S}_{\text{env}}(q, p) = \lim_{dt \rightarrow 0} \frac{1}{dt} \int_{-\infty}^{+\infty} dq' \int_{-\infty}^{+\infty} dp' G_c(q', p' | q, p; dt) dS_{\text{env}}(q', p' | q, p; dt). \quad (39)$$

Since for $dt \rightarrow 0$ the integral is dominated by short paths we can Taylor-expand the differential entropy production by

$$dS_{\text{env}}(q', p' | q, p; dt) = \sum_{i,j=0}^{\infty} \sigma_{ij}(q, p; dt) (q' - q)^i (p' - p)^j. \quad (40)$$

Inserting this expansion back into Eq. (39) we can rewrite the local entropy production as

$$\dot{S}_{\text{env}}(q, p) = \lim_{dt \rightarrow 0} \frac{1}{dt} \sum_{i,j=0}^{\infty} \sigma_{ij}(q, p; dt) M_{ij;c}(q, p; dt), \quad (41)$$

where $M_{ij;c}$ denotes the moments

$$M_{ij;c}(q, p; dt) = \int_{-\infty}^{+\infty} dq' \int_{-\infty}^{+\infty} dp' G_c(q', p' | q, p; dt) (q' - q)^i (p' - p)^j, \quad (42)$$

As we are interested in taking the limit $dt \rightarrow 0$ in Eq. (41) it is sufficient to compute $\sigma_{ij}(q, p; dt)$ and $M_{ij;c}(q, p; dt)$ only to first order in dt .

Calculation of the moments for an overdamped particle: Let us now compute the local entropy production rate for the overdamped particle

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -V'(q) - \gamma(p)p + \Gamma(p)\xi(t). \end{aligned} \quad (43)$$

We calculated the moments $M_{ij;c}(q, p; dt)$ in Eq. (42) by standard methods using a two-fold application of the saddle point method combined with a limit $\epsilon \rightarrow 0$, finding the following results:

$$M_{00;c} = 1 + \mathcal{O}(dt) \quad (44)$$

$$M_{01;c} = \left(-p\gamma(p) - V'(q) \right) dt + \mathcal{O}(dt^2) \quad (45)$$

$$M_{02;c} = \Gamma(p)^2 dt + \mathcal{O}(dt^2) \quad (46)$$

$$M_{ij;c} = \mathcal{O}(dt^{i+1}) \quad (i, j > 0) \quad (47)$$

Remarkably, the parameter c in the short-time propagator in Eq.(42) does not appear in the relevant leading order terms but only in higher-order corrections.

Now the local entropy production rate (41) can be calculated directly, and it turns out that both the approach by Spinney and Ford and our variant yield exactly the *same* result, namely,

$$\begin{aligned}\dot{S}_{\text{env}}(q, p) = & -\gamma(p) + \frac{2p^2\gamma(p)^2}{\Gamma(p)^2} - p\gamma'(p) \\ & + \frac{4p\gamma(p)\Gamma'(p)}{\Gamma(p)} + \Gamma'(p)^2 - \Gamma(p)\Gamma''(p).\end{aligned}\quad (48)$$

In order to obtain the global entropy production rate averaged over the whole phase space as a function of time, this expression has to be integrated weighted by the actual probability distribution (see Eq. 16)

$$\dot{S}_{\text{env}}(t) = \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp p(q, p, t) \dot{S}_{\text{env}}(q, p). \quad (49)$$

Entropy production in thermal equilibrium: Let us finally consider the special case of thermal equilibrium. For a system where $\gamma(p)$ and $\Gamma(p)$ obey the generalized Einstein equation (19), which is synonymous for transition rates obeying detailed balance, the differential entropy production according to Spinney and Ford and the present paper is given by

$$dS_{\text{env}}^{\text{SF}} = -\beta p (dp + pV'(q)dt) - \frac{\beta}{2}\Gamma(p)^2 dt \quad (50)$$

$$dS_{\text{env}}^{\text{HF}} = -\beta p (dp + pV'(q)dt). \quad (51)$$

As one can see, only the second version vanishes along the deterministic trajectory $\dot{p} = -V'(q)$. Nevertheless the local entropy production rate

$$\dot{S}_{\text{env}}(q, p) = -\frac{1}{2}\beta\Gamma(p)^2 + \frac{1}{2}\beta^2 p^2 \Gamma(p)^2 - \beta p \Gamma(p)\Gamma'(p) \quad (52)$$

turns out to be the same in both cases. Note that this quantity may be nonzero even in equilibrium since the entropy production is a fluctuating quantity. However, as expected the mean entropy production rate (49) integrated over phase space is in fact zero in the stationary state (17), i.e.

$$\dot{S}_{\text{env}}^{\text{eq}} = \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \frac{1}{Z} e^{-\beta\left(\frac{p^2}{2} - V(q)\right)} \dot{S}_{\text{env}}(q, p) = 0. \quad (53)$$

This can be shown by splitting the last term in (52) into two equal halves and then rewriting one of them by parts. This is plausible since for equilibrium system, including those with generalized Einstein relations, the average entropy production rate in the environment should be zero.

5 Conclusion

In this paper we have proposed a definition of the differential entropy production along a stochastic trajectory in continuous phase space systems with inertia. Our approach does not depend on the distinction between even and odd variables, instead it requires to split up the dynamics into an underlying deterministic and a stochastic part. The key idea is to consider a system that moves along its deterministic trajectory as remaining in the same state and that only jumps between different Hamiltonian orbits produce entropy in the environment. In other words, instead of points in phase space we identify the underlying Hamiltonian orbits as the microstates of the system.

Following these physically motivated ideas we arrive at an expression for the differential entropy production $dS_{\text{env}}^{\text{HF}}(q, p, dq, dp; dt)$ which differs from a previously studied expression proposed by Spinney and Ford. In particular, it vanishes along the underlying Hamiltonian orbits.

The apparent contradiction can be resolved by computing the local entropy production rate $\dot{S}_{\text{env}}(q, p)$ which turns out to be the same in both cases. This demonstrates that the notion of differential entropy production incorporates an element of ambiguity. As there are various short-time propagators generating the same time evolution, we arrive at the main conclusion that various versions of the differential entropy production generate, when integrated, the same local entropy production rate. A systematical investigation of the full range of this ambiguity would be desirable.

Entropy production in thermal equilibrium:

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A Separating Hamiltonian and non-Hamiltonian parts

The principle behind separating Hamiltonian and non-Hamiltonian parts of the dynamics is simple: upon time reversal, a Hamiltonian particle reaches its origin again. If it does not, then the discrepancy is precisely the non-Hamiltonian part of the equations. The most general case reads (with $x = q$ or p).

$$\dot{x} = f_x(q, p) + \Gamma_x(q, p)\xi_x(t) \quad (54)$$

We are now interested in the non-Hamiltonian quantities \dot{q}_Δ , \dot{p}_Δ , so that equations

$$\dot{x}_H = \dot{x} - \dot{x}_\Delta \quad (55)$$

form a Hamiltonian system. The procedure to obtain these quantities is straightforward:

1. Calculate $x(t + dt/2)$.
2. Reverse the system's dynamics by substituting $p \rightarrow -p$.
3. Evolve the for another $dt/2$, starting at the previously reached end point, but with the new dynamics.
4. The end position is $x(t + dt)$, from which $x_\Delta = x(t + dt) - x(t)$ can be determined. (\dot{x}_Δ is in the limit $dt \rightarrow 0$.)

For example, this procedure applied to the underdamped particle discussed in the present work

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -V'(q) - \gamma(p)p + \Gamma(p)\xi(t) \end{aligned} \quad (56)$$

results in

$$\dot{q}_H = p \quad \dot{q}_\Delta = 0 \quad (57)$$

$$\dot{p}_H = -V'(q) \quad \dot{p}_\Delta = -\gamma(p)p + \Gamma(p)\xi(t) . \quad (58)$$

Note that this approach is quite general and can be applied to more complicated systems, in which the separation may not be as clear.

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